

Optimal conversion of Bose-Einstein condensed atoms into molecules via a Feshbach resonance

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In many experiments involving conversion of quantum degenerate atomic gases into molecular dimers via a Feshbach resonance, an external magnetic field is linearly swept from above the resonance to below resonance. In the adiabatic limit, the fraction of atoms converted into molecules is independent of the functional form of the sweep and is predicted to be 100%. However, for non-adiabatic sweeps through resonance, Landau-Zener theory predicts that a linear sweep will result in a negligible production of molecules. Here we employ a genetic algorithm to determine the functional time dependence of the magnetic field that produces the maximum number of molecules for sweep times that are comparable to the period of resonant atom-molecule oscillations, $2\pi\Omega_{Rabi}^{-1}$. The optimal sweep through resonance indicates that more than 95% of the atoms can be converted into molecules for sweep times as short as $2\pi\Omega_{Rabi}^{-1}$ while the linear sweep results in a conversion of only a few percent. We also find that the qualitative form of the optimal sweep is independent of the strength of the two-body interactions between atoms and molecules and the width of the resonance.

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I. INTRODUCTION

Unlike alkali atoms, molecules can not be directly cooled using the laser cooling techniques that led to Bose-Einstein condensation because of the complex rotational-vibrational spectrum of the molecules. As a result, two-photon Raman photoassociation and Feshbach resonances have become the standard tools to create translationally cold molecules starting from ultra-cold atomic gases. The conversion of a macroscopic number of quantum degenerate atoms into molecular dimers starting from either a Bose-Einstein condensate [1, 2, 3, 4] or a Fermi gas [5, 6, 7, 8] has been observed by several experimental groups using a Feshbach resonance. This work culminated in the formation of a molecular Bose-Einstein condensate (MBEC) [9, 10].

Until recently the field of molecular optics was in the same state as atom optics before BEC. Diffraction and interferometry had been demonstrated [11] but there was no source of high density phase coherent monoenergetic molecules analogous to a laser that could be used to observe nonlinear and quantum optical effects. Indeed, the ability to now coherently produce molecules with a high phase space density opens up new avenues of research in the area of matter-wave optics such as lasing and matter wave amplifications with molecular fields, nonlinear mixing of atomic and molecular matter waves, and the generation of entangled atoms by ‘down conversion’ of the molecules. Recent experiment have shown the phase coherent and momentum conserving nature of matter wave second harmonic generation [12].

From the perspective of atom optics, the conversion of atoms into molecules via a Feshbach resonance or photo-association is the matter-wave analog of second harmonic generation of photons in a nonlinear crystal with a $\chi^{(2)}$ susceptibility, which has been used to cre-

ate entangled photon states. From another perspective, these methods can be viewed as the first step towards ‘quantum super-chemistry’ where chemical reactions occur in a controllable phase coherent manner and exhibit novel quantum features such as interference and bosonic stimulation [13]. Also, the ability to create molecules with permanent dipole moments using a heteronuclear Feshbach resonance [14] opens up the possibility of studying bosonic systems with anisotropic interactions [15]. Dipolar molecules can be stored in electrostatic storage rings [16] that have an area that is twenty five times larger than the largest neutral atom magnetic storage ring [17]. Storage rings for dipolar molecules therefore have the potential to be used for high precision rotation sensors based on the Sagnac effect, which is proportional to area enclosed by the ring.

Whatever the reason for creating ultracold molecules, it is highly desirable to have an efficient means of production. While the molecules created via a Feshbach resonance are translationally very cold, they are vibrationally very hot and can decay to lower lying vibrational states via exoergic inelastic collisions with atoms or other molecules. For an atomic BEC, the molecular two-body decay rates are of the order $10^{-11} - 10^{-10} \text{ cm}^3/\text{s}$, which gives a lifetime of $100 \mu\text{s}$ for a typical atomic density [3, 18, 19]. It is therefore important to be able to create the molecules as quickly as possible so that experiments can be performed on them before they are lost from the system. (In this paper, we will not consider molecules created from an atomic Fermi gas, which can have lifetimes on the order of a second due to Pauli blocking of collisions [20].)

In experiments using Feshbach resonances in atomic BECs, adiabatic rapid passage is used to convert atoms into molecules by ‘slowly’ varying an external magnetic field from above resonance, where the energy of the

molecular state lies above that of the atoms to below resonance, where molecules are the stable ground state. When the magnetic field strength is swept linearly across the Feshbach resonance, the atomic and molecular populations can be predicted by the Landau-Zener (LZ) formulae for a two-level quantum system [21]. If there are initially no molecules at $t \rightarrow -\infty$, the probability at $t \rightarrow +\infty$ of a pair of atoms remaining unconverted, P_{atom} , and of being converted into molecules, $P_{molecule}$, is given by [21],

$$P_{atoms} = e^{-2\pi\delta_{LZ}} \quad (1)$$

$$P_{molecules} = 1 - e^{-2\pi\delta_{LZ}} \quad (2)$$

$$\delta_{LZ} = \Omega_{Rabi}^2/4|\dot{\Delta}| \quad (3)$$

where Ω_{Rabi} is the Rabi frequency coupling the two states and $\Delta(t) = |\dot{\Delta}|t$ is the energy difference (detuning) between the two states. The Landau-Zener (LZ) factor δ_{LZ} is the main parameter that describes the atom-molecule conversion in theoretical models [22].

In the absence of decay of the atoms and molecules, 100% molecular conversion is expected from the LZ theory for sufficiently small $|\dot{\Delta}|$. If the detuning varies slowly enough to satisfy the adiabatic condition, $\delta_{LZ} > 1$, the initial atomic BEC will adiabatically evolve into a molecular BEC. In reality, the conversion rates are always much smaller than that predicted by LZ theory due to molecular vibrational decay [18, 19]. Experiments with atomic BECs have yielded molecular conversion efficiencies of only $\sim 5 - 10\%$ with a large fraction of the atoms being lost during the sweep [2, 4]. The missing fraction of atoms in the experiments are attributed to vibrational decay of the molecules, although spontaneous dissociation of molecules caused by inelastic spin flips has been shown to be important in ^{85}Rb [24]. This was recently confirmed by experiments in an optical lattice where ^{87}Rb dimers were created with 95% efficiency on lattice sites initially containing only two atoms so that vibrational decay of the resulting molecule was impossible [25].

Motivated by the need to create molecules faster than atom and molecule loss rates, we have explored atom-molecule conversion via a Feshbach resonance in the non-adiabatic regime. The sweep times that we are primarily interested in are shorter than the molecular lifetimes and therefore we ignore decay processes. To this end we have employed a genetic algorithm to determine the magnetic

field sweep that maximizes the fraction of atoms converted into molecules for sweeps as short as $2\pi\Omega_{Rabi}^{-1}$. We find that the optimal sweep shows a conversion efficiency in excess of 95% when the linear sweep results in a conversion of only a few percent. Moreover, the general form of the optimal sweep is independent of the strength of the resonance and the strength of the two-body interactions between atoms and molecules. These results indicate that higher conversion efficiencies could be obtained in experiments with the added bonus of longer times to perform experiments on the molecules. A recent experiment on a Cs atomic BEC showed that up to 30% of the atoms could be converted into molecules using a sweep through resonance that is similar to the one we propose here [26]. However, the duration of their sweep is much longer than what we consider here and can be considered adiabatic.

This paper is organized as follows. In section II we explain our physical model and in section III we discuss the genetic algorithm used. In section IV we compare the results obtained from the genetic algorithm with a linear LZ sweep through resonance. Section V presents some conclusions and future directions for this work.

II. PHYSICAL MODEL

A Feshbach resonance is a collisional resonance between a pair of free colliding atoms and a molecular bound state of those atoms. The coupling between the atomic and molecular states is due to the hyperfine interaction, which can result in spin flip of the electrons [27]. The colliding atom state is usually referred to as the open channel while the molecular state is known as the closed channel since it can only be accessed by a spin flip of one of the atoms. Because the atomic and molecular states have different magnetic moments, the energy difference of the atoms and molecules can be tuned using an external magnetic field.

At zero temperature, a weakly interacting BEC of atoms can be described by the semi-classical Gross-Pitaevskii equation. These equations can readily be extended to include a molecular BEC produced by coherent interconversion of atoms into molecules via a Feshbach resonance [22, 27, 28],

$$i\hbar\dot{\phi}_1 = \left(\frac{\hbar^2}{2m_1}\nabla^2 + V_1(\mathbf{x}) + U_{11}|\phi_1|^2 + U_{12}|\phi_2|^2 \right) \phi_1 + \chi\phi_1^*\phi_2 \quad (4)$$

$$i\hbar\dot{\phi}_2 = \left(-\hbar\Delta(t) + \frac{\hbar^2}{2m_2}\nabla^2 + V_2(\mathbf{x}) + U_{22}|\phi_2|^2 + U_{12}|\phi_1|^2 \right) \phi_2 + \chi\phi_1^2/2 \quad (5)$$

where ϕ_1 is the atomic BEC wave function and ϕ_2 that

of the molecules. Here, m_i are the masses and $V_i(\mathbf{x})$

the external trapping potential of the atoms ($i = 1$) and molecules ($i = 2$). The two-body interaction is given by a contact potential, $V(\mathbf{r} - \mathbf{r}') = U_{ij}\delta(\mathbf{r} - \mathbf{r}')$, with the coupling constants $U_{ij} = 2\pi\hbar^2 a_{ij}/m_{ij}$ where a_{11} is the atom-atom s-wave scattering length, a_{22} the molecule-molecule scattering length, a_{12} the atom-molecule scattering length, and $m_{ij} = m_i m_j / (m_i + m_j)$. χ is the coupling between the open channel and the closed channel defined by $\chi = [2\pi\hbar^2 a_{11} \Delta\mu \Delta B / m]^{1/2}$, where $\Delta\mu$ is difference between magnetic moments of an atomic pair and a molecule and ΔB is the width of resonance [27].

$\hbar\Delta(t) = \Delta\mu(B(t) - B_0)$ is the Zeeman energy difference between the molecules and atoms such that B_0 is the magnetic field strength at which the energy of the molecule equals the open channel collision threshold. For $\Delta(t) < 0$ the atoms are the lowest energy state while for $\Delta(t) > 0$, the molecular state is the lowest energy state of the system. Although we ignore vibrational decay of the molecules in our calculations, it can be easily included by making the substitution $\Delta(t) \rightarrow \Delta(t) - i\kappa_a |\phi_1(t)|^2 - i\kappa_m |\phi_2(t)|^2$ [27].

Unless stated otherwise we used the following values for the two-body interactions, $U_{11}/\hbar = 4.96 \times 10^{-17} \text{m}^3/\text{s}$, $U_{12}/\hbar = -6.44 \times 10^{-17} \text{m}^3/\text{s}$, $U_{22}/\hbar = 2.48 \times 10^{-17} \text{m}^3/\text{s}$ corresponding to the scattering lengths of an ^{87}Rb condensate. For the atom-molecule coupling constant we use $\chi/\hbar = 1.91 \times 10^{-5} \text{m}^{3/2}/\text{s}$ in all of our simulations [22]. We also take $V(\mathbf{x}) = 0$, which implies that ϕ_1 and ϕ_2 will be spatially homogenous. This is justified even for trapped gases in the local density approximation [29].

In this paper, we are interested in the functional form of $\Delta(t)$ that optimizes the conversion of atoms into molecules starting from the initial condition $\phi_1 = \sqrt{n_0}$, $\phi_2 = 0$, and $\Delta(t) < 0$. We also impose the constraint that the initial, $\Delta(-T/2)$, and final, $\Delta(T/2)$, values of the detuning, and the sweep time, T , are fixed. We employ a genetic algorithm to find the optimal sweep for range of different T . The conversion efficiency of the sweep is given by the probability that a pair of atoms becomes a molecule, $P_{\text{molecule}} = 2|\phi_2(T/2)|^2/n_0$.

III. GENETIC ALGORITHM

Genetic algorithms (GAs) have become a widely used tool for solving optimization problems that depend on a large number of variables [30]. These multidimensional optimization techniques proceed by parameterizing an objective function in terms of a finite set of coefficients, the chromosome. The genetic algorithm operates on a set of chromosomes, which represent the members of a population.

The goal is to find the chromosome that is the global minimum of the objective function. In order to find the optimal chromosome, GAs employ Darwin's principle of survival of the fittest. At each generation, the chromosomes in the population compete with each other for survival. The members of the population that do the

best job of minimizing the objective function, survive to the next generation while those that do a poor job are eliminated. The surviving members are allowed to produce offspring for the next generation by some prescribed mating rules that mix elements from their chromosomes (crossover). Random mutations are also introduced into the offspring chromosomes at each generation. This process repeats itself until the change in the optimum solution between successive generations is less than some threshold value.

We want to optimize the molecular fraction obtained by sweeping $\Delta(t)$ from $\Delta(-T/2) = -|\Delta_0|$ to $\Delta(T/2) = |\Delta_0|$. The detuning is parameterized in terms of either a power series,

$$\Delta(t) = \sum_{n=1}^N C_n t^n \quad (6)$$

or a Fourier series,

$$\Delta(t) = \sum_{n=1}^N B_n \sin\left(\frac{n\pi t}{T}\right). \quad (7)$$

The coefficients C_n or B_n are the elements of a chromosome, where we used $N = 160$ coefficients for Eq. (6) and $N = 320$ coefficients for Eq. (7). The initial population consists of $N_{\text{pop}} = 20$ randomly chosen chromosomes. We solve the coupled Gross-Pitaevskii equations, Eqs. 4 and 5, for each detuning function in the current generation. The half of the population that produces the largest fraction of molecules are kept and allowed to breed to produce $N_{\text{pop}}/2$ new chromosomes while the other half are discarded.

Crossover is accomplished by choosing pairs of chromosomes and representing them as binary strings. A random point in the strings is chosen and all information to the right of that point is swapped. The mutation operator randomly flips the value of single bits within the binary strings of the offspring chromosome. This process of selection, crossover, and mutation continues until the difference in optimal conversion efficiency between 50 successive generations is less than 0.1%. This stopping condition is because the GA can become stuck for several generations at local minima of the objective function.

IV. NUMERICAL RESULTS

The conversion efficiencies of atoms into molecules determined by the GA are characterized by the initial and final values of detuning functions ($|\Delta_0|$), sweep time (T), and the mean field energy shifts for the atoms and molecules, which are proportional to U_{11} , U_{12} , and U_{22} . In order to make our results independent of the strength of the resonance, all times and frequencies are scaled relative to the initial Rabi frequency, $T_{\text{Rabi}}/2\pi = \Omega_{\text{Rabi}}^{-1} = \hbar/\chi\sqrt{n_0}$. However, to provide a feeling for the relevant time scales, we note that $T_{\text{Rabi}} = 16\mu\text{s}$ for the initial

atomic density of $n_0 = 4 \times 10^{14} \text{cm}^{-3}$ that we use in our simulations.

We first investigated the molecular conversion efficiency as a function of magnetic field sweep time with $|\Delta_0| = 50\Omega_{\text{Rabi}}$. This initial value of the detuning is large enough to decouple the atoms and molecules. The circles and squares in Fig. 1(a) indicate the conversion efficiency for a linear sweep and optimal sweep, respectively. For long enough sweep times, $\tau \equiv T/T_{\text{Rabi}} > 100$, both sweeps show very large conversion efficiencies of around 95% or more. In this limit, the sweeps are adiabatic and the conversion efficiency is therefore independent of the shape of the detuning function.

As τ is decreased, the optimal sweep is still able to convert almost all atoms into molecules while the conversion efficiency of a linear sweep decreases rapidly. For $\tau \sim 1$, the conversion efficiency of a linear sweep is only a few percent. This is easily understood by noting that as τ decreases the linear sweep is no longer adiabatic. For $\tau = 100$, $\delta_{LZ} = 1.57$ and according to Eq. (2), $P_{\text{molecule}} = 0.99$ while for $\tau = 1$ the LZ factor decreases to $\delta_{LZ} = 0.015$ giving a molecular fraction of only $P_{\text{molecule}} = 0.089$. These values agree qualitatively with the numerical solution of the GP equations in Fig. 1(a), which indicates that the LZ factor is the main parameter controlling the atom-molecule conversion. By contrast, the optimal sweeps show excellent conversion even for very small sweep times. For comparison the optimal sweep gives 98.48% and 99.82% conversion for $\tau = 1$ and 2, while the linear sweep gives 6.74% and 10.64%, respectively.

Fig. 2 shows the optimal sweep for $\tau = 2$ using both Eq. (6) and (7). The power series and the Fourier series result are almost identical except for the small noise fluctuations present in the Fourier series. The noise in the Fourier series GA varied from run to run but always had an average amplitude less than Ω_{Rabi} . The noise was the result of the high frequency terms in the Fourier series, $n\pi/T \gg \Omega_{\text{Rabi}}, |\Delta_0|$, which oscillate much faster than all other time scales in the Gross-Pitaevskii equations. We therefore do not expect these fluctuations to have any appreciable effect on the dynamics. These high frequency terms needed to be included in $\Delta(t)$ to produce the large slope at the beginning and end of the sweep.

To study the effect of these fluctuations, we superimposed randomly generated noise on top of the optimal sweep obtained from the power series, Eq. (6). The average amplitude of the noise was varied between $0.01\Omega_{\text{Rabi}}$ and $100\Omega_{\text{Rabi}}$. We then calculated the conversion efficiency of the power series detuning with the added noise. For noise amplitudes less than Ω_{Rabi} there was no noticeable change in the conversion efficiency or the dynamics of the atom-molecule conversion. While noise amplitudes larger the Ω_{Rabi} significantly effect the conversion dynamics and efficiency. This indicates that as long as the size of the fluctuations are small enough to not shift the two states into or out of resonance with each other, there will be no observable effect.

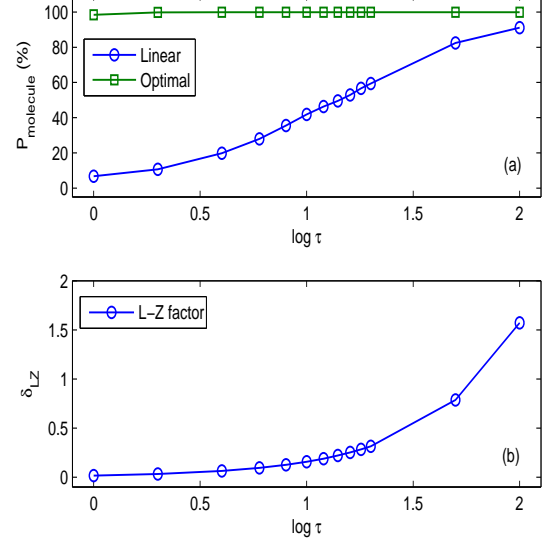


FIG. 1: (Color online)(a) Fraction of atoms converted into molecules as a function of $\log_{10} \tau$ where τ is the dimensionless magnetic field sweep time, $\tau = T/T_{\text{Rabi}}$ for fixed initial and final detunings $\Delta(-\tau/2) = -\Delta(\tau/2) = -|\Delta_0| = -50\Omega_{\text{Rabi}}$. Here we chose $T_{\text{Rabi}} = 1.6465 \times 10^{-5} \text{s}$. The circles and squares indicate the conversion rate for the linear and optimal sweeps, respectively. (b) Landau-Zener factors, δ_{LZ} , for linear sweep.

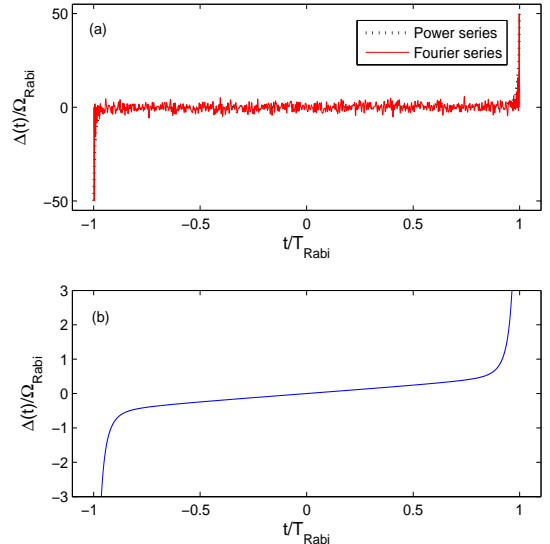


FIG. 2: (Color online) (a) The optimal sweep for $\tau = 2$. The dotted line is the optimal sweep obtained from Eq. (6) while the solid line is that obtained from Eq. (7). (b) Closeup of the optimal sweep obtained from Eq. (6) for the power series.

In order to understand why the optimal sweep is able to achieve such high conversion efficiencies even for very small τ , we plot in Fig. 3 the *instantaneous* Landau-Zener factor $\delta_{LZ}(t) = \Omega_{Rabi}^2(t)/4|\dot{\Delta}(t)|$ where $\Omega_{Rabi}(t) = \chi|\phi_1(t)|$ and $\Delta(t)$ is the GA optimal sweep. At the beginning and end of the sweep $\delta_{LZ}(t) \ll 1$, which indicates that the sweep is non-adiabatic. However, at these times the detuning is so large that the atoms and molecules are decoupled. It is only for $\Delta(t) < \Omega_{Rabi}(t)$ that the atom-molecule system is resonant and atoms can be converted into molecules. At these times $\delta_{LZ}(t) > 1$, which implies that the system is actually adiabatic.

As one can see from Fig. 2, the optimal sweep rapidly goes from far off resonance to close to resonance and once near resonance the sweep rate slows down to maintain adiabaticity. By using the narrow time interval at the beginning and end of the sweep where the detuning function changes the fastest, Δt , one can estimate the frequency bandwidth of the sweep, $\Delta E/\hbar \approx 1/\Delta t$, to be $\approx 4.5 MHz$. This is several orders of magnitude smaller than the typical energy spacing between molecular vibrational levels in the closed channel. Consequently, the coupling between atoms and more than one molecular state can be ignored.

At the same time the gradient of the detuning is large enough to prevent nonadiabatic oscillations, as one can see from Fig. 4(a). On the other hand the linear sweep results in nonadiabatic oscillations close to resonance that are the result of the coupling between the dressed states that is proportional to $\dot{\Delta}(t)/\Omega_{Rabi}$. In the optimal sweep the atom-molecule conversion occurs gradually over almost the entire sweep, while the conversion is limited to a very small window of approximately $t \approx 0$ to $t \approx 0.1\tau$ for the linear sweep. The optimal sweep is similar to the switching scheme demonstrated in [26] where the magnetic field was held at a fixed value close to the resonance for a certain time ($t \geq 15ms$). The switching scheme produced more molecules than the linear sweep because the atoms spent more time within the line width of the resonance where molecules can be created. However, we emphasize that their hold times near resonance were several orders of magnitude longer than the nonadiabatic sweep times we consider here.

To see whether the form of the optimal detuning was unique to Eqs. (4) and (5) or were universal to two-state systems, we tested our GA on a two-level quantum mechanical system with the Hamiltonian,

$$H = \hbar \begin{pmatrix} 0 & \Omega_{Rabi} \\ \Omega_{Rabi} & -\Delta(t) \end{pmatrix} \quad (8)$$

Fig. 5 shows the populations of the two levels $|a\rangle$ and $|m\rangle$ with all of the population initially in $|a\rangle$. The dynamics of the conversion of $|a\rangle$ into $|m\rangle$ is qualitatively the same as the atoms and molecules as is the shape of the optimal detuning function. This indicates that the general form of the optimal $\Delta(t)$ is generic to any two state system.

The mean field energy shifts of the atoms ($U_{11}|\phi_1|^2$, and $U_{12}|\phi_2|^2$) and molecules ($U_{22}|\phi_2|^2$ and $U_{12}|\phi_1|^2$)

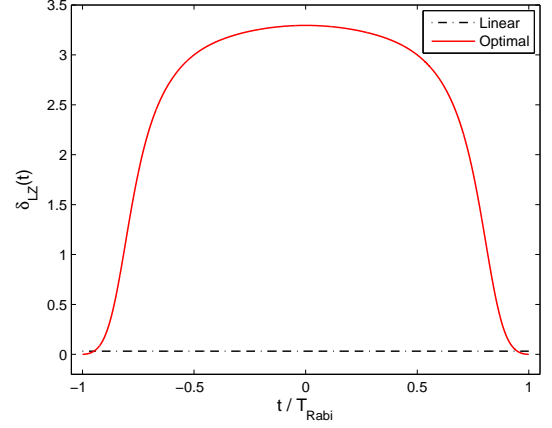


FIG. 3: (Color online) Instantaneous Landau-Zener factor, $\delta_{LZ}(t)$ for the optimal sweep (solid line) and linear sweep (dot-dashed line). The sweep time is $t = 2T_{Rabi}$

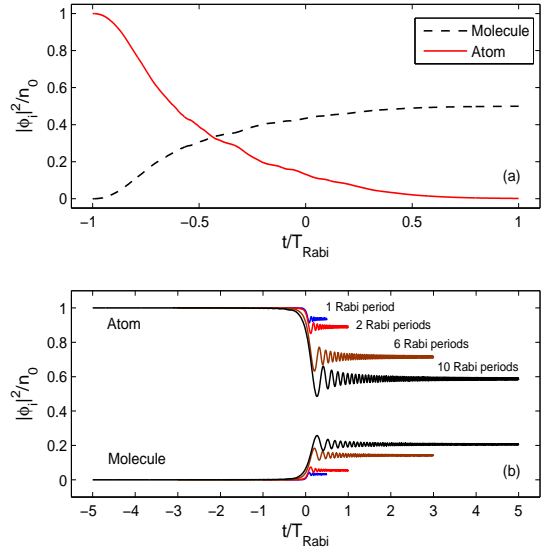


FIG. 4: (Color online) (a) Atomic, $|\phi_1|^2/n_0$, (solid line) and molecular, $|\phi_2|^2/n_0$, (dashed line) fractions from the optimal sweep for $\tau = 2$. (b) Atomic and molecular fraction obtained from linear sweep for $\tau = 1, 2, 6, 10$.

modifies the energies of the atom and molecules so that the difference in the chemical potentials between the atoms and molecules, $\Delta\mu = \mu_{molecule} - \mu_{atom}$, to zeroth order in χ is [31],

$$\Delta\mu = -\hbar\Delta(t) + U_{22}|\phi_2|^2 - U_{11}|\phi_1|^2 + U_{12}(|\phi_1|^2 - |\phi_2|^2) \quad (9)$$

Consequently, even when $\Delta(t) = 0$ the energy difference between the atoms and molecules is not zero.

In order to test the effect of the mean field shifts on the conversion process, we consider a range of possible values for the coupling constants U_{ij} to see how sensitive

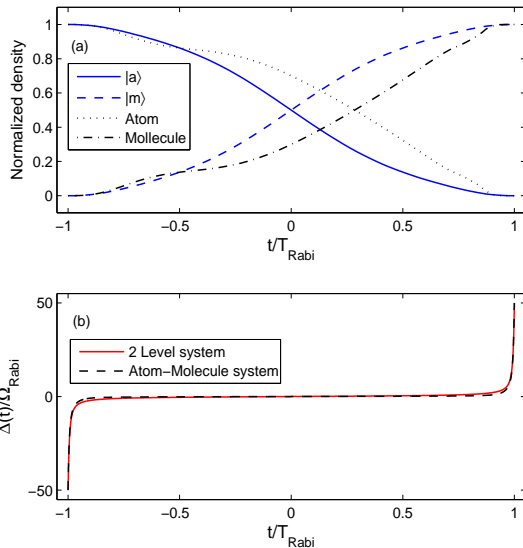


FIG. 5: (Color online)(a) Populations of two level quantum system, $|a\rangle$ (solid line) and $|m\rangle$ (dashed line) obtained from optimal sweep through resonance for $\tau = 2$. Also shown are atomic, $|\phi_1|^2/n_0$, (dotted) and molecular, $2|\phi_2|^2/n_0$, (dashed dot) fractions for with $U_{11} = U_{12} = U_{22} = 0$ and initial Rabi frequency chosen to match that of the two level system. (b) Optimal sweep, $\Delta(t)$, obtained from Eq. 6 for two level system (solid line). For comparison, the optimal detuning for the atom-molecule system is also shown (dashed line).

the shape of the optimal sweep and the conversion efficiency is to variations of these parameters. We took the coupling constants to be either 0.1, 1, or 10 times bigger than the values given in Sec. II, which we denote here by $U_{ij}^{(0)}$. The maximum conversion efficiency for each of the 27 different combination of values are shown in Fig. 6. The numbers in parentheses represent the relative magnitudes of the three coupling constants. For example, (1, 10, 0.1) means that $U_{11} = U_{11}^{(0)}$, $U_{12} = 10U_{12}^{(0)}$, and $U_{22} = 0.1U_{22}^{(0)}$.

In all cases, the optimal sweep shows very good conversion ($\geq 98\%$) compared to less than 5% for the linear sweep even for very short sweep times. For instance, with $U_{11} = 10U_{11}^{(0)}$, the optimal sweep still shows better conversion than the linear sweep giving for example $\sim 99\%$ conversion compared to $< 5\%$ for $\tau = 2$. To understand this we note that from Fig. 4(a), most of the conversion takes place at the beginning of the sweep, $t/\tau \approx -1.0$ to -0.5 where the atomic density is much larger than the molecular density. At these times the molecular energy lies above that of the atoms, $-\hbar\Delta(t) > 0$ and the atomic mean field $U_{11}|\phi_1|^2$ shift reduces $\Delta\mu$.

As the U_{ij} are varied, the qualitative form of the optimal detuning are the same as Fig. 2. There are, however, quantitative variations in the slope for different U_{ij} as can be seen in Fig. 7. We tested the optimal detuning for

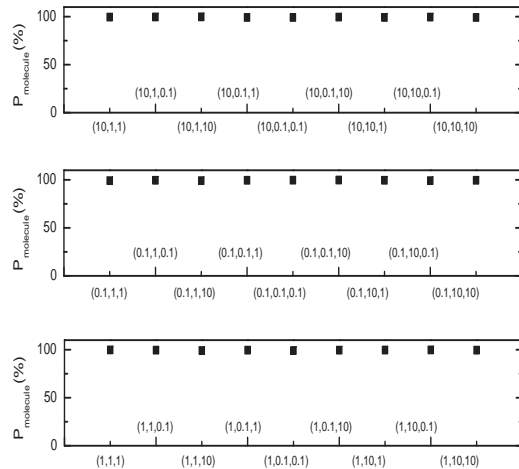


FIG. 6: Molecular fraction as a function of non-linear interaction terms for $\tau = 2$. The numbers in parentheses indicate relative magnitude of the mean field coupling constants U_{11} , U_{12} , and U_{22} , respectively. For instance, (10, 10, 0.1) means $U_{11} = 10U_{11}^{(0)}$, $U_{12} = 10U_{12}^{(0)}$, and $U_{22} = 0.1U_{22}^{(0)}$.

each of the the 27 combination of parameters denoted by $\Delta_{(l,m,n)}(t)$, on the other 26 combination of parameters. In all cases the $\Delta_{(l,m,n)}$ performed significantly better when applied to the other combination of parameters than the linear sweep. These results imply that the optimal detuning calculated for any set of values of the two-body interaction can be used to convert atoms into molecules with greater efficiency than a linear sweep.

V. DISCUSSION

Very close to resonance, mean field theory breaks down due to the divergence of the scattering length and higher order quantum correlations can become important [28]. These higher order correlations have been shown to be important for time dependent experiments such as in Ref. [1] where the atoms and molecules are placed in a coherent superposition state and allowed to evolve freely [32]. However, theoretical calculations that compare mean field theory and microscopic quantum calculations that account for higher order correlations have been shown to give nearly identical results for the molecular conversion efficiency for downward magnetic field sweeps through a resonance [22, 28]. Although these calculations were for linear sweeps, the agreement was very good for a range of $\dot{\Delta}$ that included non-adiabatic sweeps for which Landau-Zener theory gives $P_{\text{molecules}} \ll 1$. These results support our use of mean field theory to model the atom-molecule conversion. It would, however, be of great interest to extend the work of Ref. [22] and compare mean

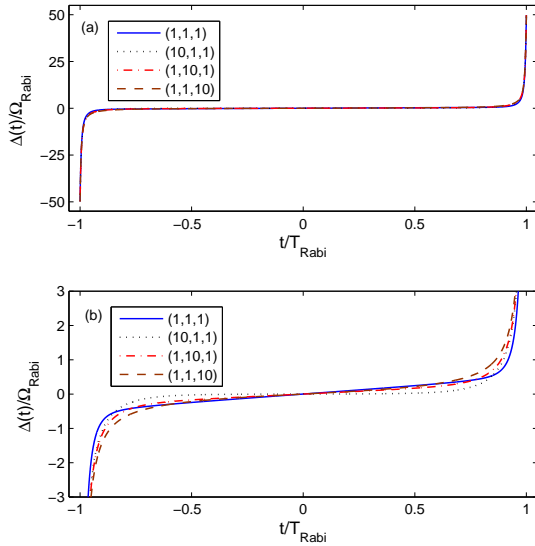


FIG. 7: (Color online) Optimal detuning function for several different values of U_{11} , U_{12} , and U_{22} .

field theory to quantum calculations for nonlinear magnetic field sweeps.

Throughout this paper we have ignored the effect of the decay of the molecules. If we assume a two-body inelastic decay rate of $5 \times 10^{-11} \text{cm}^3/\text{s}$ [19] for molecule-molecule and atom-molecule collisions, we get a lifetime of $\tau_{\text{loss}} = 50 \mu\text{s}$ for the initial atomic density of $4 \times 10^{14} \text{cm}^{-3}$. Assuming a simple exponential decay of

the molecule number, we can estimate the fraction of molecules lost during the sweep by $\exp(-T/\tau_{\text{loss}})$. This estimate actually overestimates the molecule loss since it does not take into account the fact that τ_{loss} is not constant but instead increases as the density of the gas decreases with time. $\exp(-T/\tau_{\text{loss}})$ should, nevertheless, provide a lower bound on the fraction of molecules lost during a fast sweep. For $T = T_{\text{Rabi}} = 16 \mu\text{s}$, the molecular conversion efficiency is reduced by a factor of $\exp(-T_{\text{Rabi}}/\tau_{\text{loss}}) = 0.73$. Therefore, for a sweep time of T_{Rabi} the conversion efficiency using our optimal sweep and taking into account losses will be approximately $\exp(-T_{\text{Rabi}}/\tau_{\text{loss}}) \times 98.48\% = 72\%$.

In conclusion, we have applied a genetic algorithm to study the optimal time dependence of an applied magnetic field, $B(t)$, to convert atoms into molecules using a Feshbach resonance. Instead of the conventional linear sweep, we propose a nonlinear sweep through resonance that is characterized by a rapid approach of $B(t)$ towards the resonance position followed by a gradual change in $B(t)$ close to resonance and finally a rapid change in $B(t)$ at the end of the sweep away from the resonance. This nonlinear sweep can result in almost 99% conversion of atoms into molecules even for sweep times as short as one Rabi period. We have shown that the qualitative form of this nonlinear sweep is independent of the specific nature of the two state system. We plan to extend this work by using a genetic algorithm to optimize molecule production via two-photon Raman photoassociation. In that case both the laser frequencies and intensities of the two lasers can be treated as time dependent quantities to be optimized.

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